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## P A M Dirac meets M G Krein: matrix orthogonal polynomials and Dirac's equation

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### Abstract

The solution of several instances of the Schrödinger equation (1926) is made possible by using the well-known orthogonal polynomials associated with the names of Hermite, Legendre and Laguerre. A relativistic alternative to this equation was proposed by Dirac (1928) involving differential operators with matrix coefficients. In 1949 Krein developed a theory of matrix-valued orthogonal polynomials without any reference to differential equations. In Duran A J (1997 Matrix inner product having a matrix symmetric second order differential operator *Rocky Mt. J. Math.* **27** 585–600), one of us raised the question of determining instances of these matrix-valued polynomials going along with second order differential operators with matrix coefficients. In Duran A J and Grünbaum F A (2004 Orthogonal matrix polynomials satisfying second order differential equations *Int. Math. Res. Not.* **10** 461–84), we developed a method to produce such examples and observed that in certain cases there is a connection with the instance of Dirac's equation with a central potential. We observe that the case of the central Coulomb potential discussed in the physics literature in Darwin C G (1928 *Proc. R. Soc. A* **118** 654), Nikiforov A F and Uvarov V B (1988 *Special Functions of Mathematical Physics* (Basle: Birkhauser) and Rose M E 1961 *Relativistic Electron Theory* (New York: Wiley)), and its solution, gives rise to a matrix weight function whose orthogonal polynomials solve a second order differential equation. To the best of our knowledge this is the first instance of a connection between the solution of the first order matrix equation of Dirac and the theory of matrix-valued orthogonal polynomials initiated by M G Krein.

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## 1. Introduction

Every student of elementary quantum mechanics encounters the classical orthogonal polynomials of Hermite, Legendre and Laguerre in dealing with Schrödinger's equation for the wave function  $\psi(x, t)$ .

This equation treats space and time in an unsymmetric fashion, a feature that is not acceptable according to relativity theory. At the very beginning of the development of quantum theory a second order differential equation was proposed separately by Klein and Gordon (1926) that took care of this problem but led to negative probabilities. Schrödinger himself had arrived at this equation first but discarded it because it gave him the incorrect fine structure for hydrogen. A couple of years later P A M Dirac solved this problem by proposing a first order differential equation with *matrix coefficients*. This equation required that the electron should have spin-1/2 a fact that had been predicted by the study of atomic spectra. This as well as the agreement that Dirac's equation gave with magnetic properties of the electron as predicted a few years earlier by S Goudsmit and G Uhlenbeck gave credibility to this rather strange equation involving matrix coefficients. The equation had its problems: it predicted the existence of *anti-matter*, i.e. the existence of particles of the same mass as the electron but of positive charge, and able to interact with an electron and get both particles converted into energy. One can have sympathy for Dirac's saying 'A great deal of my work is just playing with equations and seeing what they give'. A few years later, in 1932, C Anderson found the positrons that Dirac's equation had predicted.

As mentioned earlier, Dirac's equation involves a first order differential operator with matrix coefficients acting on a four-component vector. There are alternative formulations, such as one proposed by Feynman and Gell-Mann, see [FG], where one has a pair of coupled second order equations acting on two component functions.

The radical departure that Dirac took was the introduction of matrix coefficients. At the root of this problem is the difficulty of factorizing the Laplacian in dimensions higher than one as a product of first order operators. The names of Cauchy–Riemann as well as the notion of a Clifford algebra can be heard in the background: for instance if  $D$  denotes the operator

$$\left[ \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \frac{d}{dx} + \begin{pmatrix} 0 & -1 \\ -1 & 0 \end{pmatrix} \frac{d}{dy} \right]$$

one has that  $D^2$  is the Laplacian in  $R^2$  and that the condition

$$D\psi = 0$$

is just the requirement that  $\psi = (u, v)^T$  be the real and imaginary parts of an analytic function.

Incidentally this factorization problem is not present in the case of one space dimension: Schrödinger himself invented this method in 1940, see [Sch], although the method is usually referred to as the Infeld–Hull method, see [IH]. They wrote a paper in 1951. As is often the case, none of these people were the first ones to come up with this idea: it is found in G Darboux's book on Surface Theory and is credited by him to Moutard.

The reader may feel that this digression into the *factorization problem* is not too relevant to our problem. However it is at the root of the relation between the differential equations derived in [DG1] and an instance of the Dirac equation: the case of a central potential as discussed for instance in the book by Rose, see [R] (also [NU]). This solution is due to Darwin, see [Da].

In [DG1] we observe that the solution of certain differential equations that has to be satisfied by the weight matrix  $W(t)$  is greatly aided by introducing a factorization of it in the form

$$W(t) = \rho(t)T(t)T^*(t). \quad (1.1)$$

Under certain boundary conditions satisfied by  $W$ , the differential equations for  $W$  are equivalent to the fact that  $W$  goes along with a symmetric second order differential operator of the form

$$\ell_2 = D^2 A_2 + D A_1 + D^0 A_0, \quad (1.2)$$

where  $A_2, A_1$  and  $A_0$  are matrix polynomials of degrees not bigger than 2, 1 and 0, respectively. In terms of the orthogonal polynomials with respect to  $W$ , that means that they are eigenfunctions for  $\ell_2$  (with Hermitian eigenvalues if they are orthonormal). These families of orthogonal matrix polynomials are among those that are likely to play in the case of matrix orthogonality the role of the classical families of Hermite, Laguerre and Jacobi in the case of scalar orthogonality.

For a more detailed discussion of (1.1) and (1.2) above, see section 2.

When the leading coefficient of the differential operator  $A_2(t)$  is given by  $tI$  and the scalar weight  $\rho$  is taken to be equal to a Laguerre weight,  $\rho(t) = t^\alpha e^{-t}$ , the matrix factor  $T$  in (1.1) has to satisfy a first order differential equation of the form  $T' = (A + B/t)T$ . That is precisely the form of Dirac's equation in the presence of a central Coulomb potential.

To insure that  $W$  goes along with a symmetric second order differential operator as in (1.2),  $T$  and the differential coefficients of  $\ell_2$  have to satisfy certain Hermitian condition. This condition is equivalent to the following second order differential equation for  $W$ :

$$(A_2 W)'' - (A_1 W)' + A_0 W = W A_0^*.$$

Here, we show how to build from the matrix solution  $T$  of  $T' = (A + B/t)T$ , arising from a special instance of Dirac's equation, weight matrices  $W$  going along with a symmetric second order differential operators.

It may be worth pointing out that Darwin's treatment involves another well-known special function, the confluent hypergeometric function, see (5.34) and (5.35) in page 171 of [R]. Our observations here are *not related to this special function*. On the other hand the treatment in [DL] brings up an interesting connection between a matrix-valued weight like the one discussed here and a certain matrix-valued variant of the Kummer confluent hypergeometric function.

In all the considerations below one takes our matrix-valued differential operators (with polynomial coefficients) as acting on the space of matrix-valued polynomials.

## 2. Preliminary results

By a weight matrix we mean an  $N \times N$  matrix of measures  $W$  supported in the real line satisfying

1.  $W(A)$  is positive semidefinite for any Borel set  $A \subset \mathbb{R}$ ;
2.  $W$  has finite moments of every order, and
3.  $\int P(t) dW(t) P^*(t)$  is nonsingular if the leading coefficient of the matrix polynomial  $P$  is nonsingular.

Condition (3) is necessary and sufficient to guarantee the existence of a sequence  $(P_n)_n$  of matrix polynomials orthogonal with respect to  $W$ ,  $P_n$  of degree  $n$  and with nonsingular leading coefficient. In this paper, we always consider weight matrices  $W$  that have a smooth absolutely continuous derivative  $W'$  with respect to the Lebesgue measure; if we assume that this matrix derivative  $W'$  is positive definite at infinitely many real numbers, then condition (3) above holds automatically. For other basic definitions and results on matrix orthogonality, see for instance [Be, D1, D2, K1, K2].

We are especially interested in those weight matrix  $W$  allowing for a symmetric second order differential operator of the form

$$\ell_2 = D^2 A_2(t) + D^1 A_1(t) + D^0 A_0, \quad (2.1)$$

that would have the polynomials  $P_n(t)$  as a common set of eigenfunctions.

Here  $A_2$ ,  $A_1$  and  $A_0$  are matrix polynomials of degrees less than or equal to 2, 1 and 0 (the symmetry of  $\ell_2$  is with respect to the inner product  $\int P(t) dW(t) Q^*(t)$  defined by  $W$ ). If we write  $(P_n)_n$  for a family of orthonormal polynomials with respect to  $W$ , the *symmetry* of the second order differential operator is equivalent to the second order differential equation

$$P_n''(t)A_2(t) + P_n'(t)A_1(t) + P_n(t)A_0 = \Gamma_n P_n(t) \quad (2.2)$$

for the orthonormal polynomials, where  $\Gamma_n$  are *Hermitian matrices*. These families of orthonormal polynomials are very likely going to play in the case of matrix orthogonality the crucial role that the classical families of Hermite, Laguerre and Jacobi play in the scalar one.

It turns out that, under the boundary conditions that

$$A_2(t)W(t) \quad \text{and} \quad (A_2(t)W(t))' - A_1(t)W(t), \quad (2.3)$$

vanish at each of the endpoints of the support of  $W(t)$ , the symmetry of a second order differential operator as in (2.1) with respect to a weight matrix  $W$  is equivalent to the following set of differential equations relating  $W$  and the differential coefficient of  $\ell_2$ :

$$A_2 W = W A_2^* \quad (2.4)$$

as well as

$$2(A_2 W)' = W A_1^* + A_1 W. \quad (2.5)$$

and

$$(A_2 W)'' - (A_1 W)' + A_0 W = W A_0^*. \quad (2.6)$$

Assuming that  $A_2(t)$  is a scalar, it has been proved in [DG1] that the differential equation (2.5) for  $W$  is equivalent to the fact that  $W$  can be factorized in the form  $W(t) = \rho(t)T(t)T^*(t)$ , where  $\rho$  is a scalar function and  $T$  is a matrix function satisfying a certain first order differential equation. In particular, when  $\rho$  is the classical scalar weight of Laguerre  $t^\alpha e^{-t}$ , then this first order differential equation for  $T$  is of the form

$$T'(t) = \left( A + \frac{B}{t} \right) T(t),$$

that is, of the same form as the matrix equation resulting from the Dirac equation in the case of a central Coulomb potential.

Once we take for  $W(t)$  the factorization  $W = t^\alpha e^{-t} T T^*$ , equation (2.6) is equivalent to the fact that the following matrix function has to be Hermitian ([DG1], section 4):

$$\chi(t) = T^{-1}(t) \left( (\alpha B + B^2) \frac{1}{t} + AB + BA + (\alpha + 1)A - A_0 - B + (A^2 - A)t \right) T(t). \quad (2.7)$$

### 3. Orthogonal matrix polynomials and Dirac's equation

We consider the matrices

$$A = \begin{pmatrix} 0 & 1+w \\ 1-w & 0 \end{pmatrix}, \quad B = \begin{pmatrix} -a & b \\ -b & a \end{pmatrix}.$$

These matrices are those ones that appear in equations (5.25) in [R] in connection with the Coulomb problem in the context of Dirac's equation. Note that in [NU], p 331, the matrix  $B$  has the form  $\begin{pmatrix} -1-a & b \\ -b & -1+a \end{pmatrix}$ , so that the relationship between the solution  $T$  of equations (5.25) in [R] and the solution  $R$  of equation (25) in [NU], p 331 is just  $R = T/t$ .

Since we are interested in solving the corresponding *matrix equation* for  $T(t)$  and then in checking the condition that  $\chi(t)$  given in (2.7) should be Hermitian for all values of  $t$  we need to make special choices for the parameters

$$w, a, b.$$

First of all, we need to insure that both matrices can be put simultaneously in triangular form by means of a nonsingular matrix. That is equivalent to the condition that  $A$  and  $B$  have a common eigenvector. An easy computation gives that this happens when

1.  $\sqrt{\frac{1+w}{1-w}} = -\frac{a+\sqrt{a^2-b^2}}{b}$ . In this case the common eigenvector has the form  $(z, \sqrt{\frac{1+w}{1-w}}z)$ ,  $z \neq 0$ , and it is an eigenvector of  $A$  with the eigenvalue  $\sqrt{1-w^2}$  and of  $B$  with the eigenvalue  $\sqrt{a^2-b^2}$ .
2.  $\sqrt{\frac{1+w}{1-w}} = \frac{a+\sqrt{a^2-b^2}}{b}$ . In this case the common eigenvector has the form  $(z, -\sqrt{\frac{1+w}{1-w}}z)$ ,  $z \neq 0$ , and it is an eigenvector of  $A$  with the eigenvalue  $-\sqrt{1-w^2}$  and of  $B$  with the eigenvalue  $\sqrt{a^2-b^2}$ .
3.  $\sqrt{\frac{1+w}{1-w}} = \frac{-a+\sqrt{a^2-b^2}}{b}$ . In this case the common eigenvector has the form  $(z, \sqrt{\frac{1+w}{1-w}}z)$ ,  $z \neq 0$ , and it is an eigenvector of  $A$  with the eigenvalue  $\sqrt{1-w^2}$  and of  $B$  with the eigenvalue  $-\sqrt{a^2-b^2}$ .
4.  $\sqrt{\frac{1+w}{1-w}} = \frac{a-\sqrt{a^2-b^2}}{b}$ . In this case the common eigenvector has the form  $(z, -\sqrt{\frac{1+w}{1-w}}z)$ ,  $z \neq 0$ , and it is an eigenvector of  $A$  with the eigenvalue  $-\sqrt{1-w^2}$  and of  $B$  with the eigenvalue  $-\sqrt{a^2-b^2}$ .

An easy computation shows that  $w = \pm\sqrt{a^2-b^2}/a$  (the sign depending on the cases). By referring to [NU], p 337, we see that this value of  $w$ , expressing the fact that  $A$  and  $B$  can be put simultaneously in triangular form, coincides with the lowest possible energy level in this problem.

Since all these cases can be handled in a very similar fashion, we concentrate in the first one. We hence assume that  $\sqrt{\frac{1+w}{1-w}} = -\frac{a+\sqrt{a^2-b^2}}{b}$ . Using the common eigenvector (we take  $x = 1$ ), we find the triangular matrices  $\tilde{A}$  and  $\tilde{B}$  which are similar to  $A$  and  $B$ , respectively:

$$\tilde{A} = \begin{pmatrix} 1 & 0 \\ 1 & \frac{1+w}{1-w} \end{pmatrix} \begin{pmatrix} 0 & 1+w \\ 1-w & 0 \end{pmatrix} \begin{pmatrix} 1 & 0 \\ -\frac{1-w}{1+w} & \frac{1-w}{1+w} \end{pmatrix} = \sqrt{1-w^2} \begin{pmatrix} -1 & 1 \\ 0 & 1 \end{pmatrix},$$

$$\tilde{B} = \begin{pmatrix} 1 & 0 \\ 1 & \frac{1+w}{1-w} \end{pmatrix} \begin{pmatrix} -a & b \\ -b & a \end{pmatrix} \begin{pmatrix} 1 & 0 \\ -\frac{1-w}{1+w} & \frac{1-w}{1+w} \end{pmatrix} = \begin{pmatrix} -\sqrt{a^2-b^2} & a-\sqrt{a^2-b^2} \\ 0 & \sqrt{a^2-b^2} \end{pmatrix}.$$

We are now able to integrate the differential equation

$$T' = \left( A + \frac{B}{t} \right) T, \tag{3.1}$$

and for each solution  $T$ , we can inquire whether there exists a matrix  $A_0$  such that the weight matrix  $W = t^\alpha e^{-t} T T^*$  satisfies the differential equation (2.6). Using the method developed in [DG1] (see the previous section), that is equivalent to proving that the matrix

$$\chi(t) = T^{-1}(t) \left( (\alpha \tilde{B} + \tilde{B}^2) \frac{1}{t} + \tilde{A} \tilde{B} + \tilde{B} \tilde{A} + (\alpha + 1) \tilde{A} - A_0 - \tilde{B} + (\tilde{A}^2 - \tilde{A})t \right) T(t)$$

is Hermitian.

A careful computation shows that under the assumption  $\sqrt{a^2 - b^2} = 1/2$  and  $\alpha = 0$ , there is a solution of (3.1) and a matrix  $A_0$  for which the matrix function  $\chi$  is, in fact, Hermitian. More precisely, for  $\sqrt{a^2 - b^2} = 1/2$ , we find that by taking

$$T(t) = \begin{pmatrix} t^{-1/2} e^{-\sqrt{1-w^2}t} & t^{-1/2} \left( \frac{1}{2}t + \frac{a-1}{2\sqrt{1-w^2}} \right) e^{\sqrt{1-w^2}t} \\ 0 & t^{1/2} e^{\sqrt{1-w^2}t} \end{pmatrix} \quad (3.2)$$

and

$$A_0 = \begin{pmatrix} 1 - 2\sqrt{1-w^2} & -\frac{1}{2} + \sqrt{1-w^2} \\ 0 & 0 \end{pmatrix},$$

then  $\chi$  is a diagonal matrix with entries

$$\begin{aligned} \chi_{11}(t) &= \frac{1 - (1 - 4\sqrt{1-w^2})2t + (\sqrt{1-w^2} + 1)4\sqrt{1-w^2}t^2}{4t} \\ \chi_{22}(t) &= \frac{1 - (1 - 4\sqrt{1-w^2})2t + (\sqrt{1-w^2} - 1)4\sqrt{1-w^2}t^2}{4t}. \end{aligned}$$

It turns out that the matrix function  $T$  (see (3.2)) can be factorized as follows:

$$T(t) = t^{-1/2} P(t) e^{D_{\tilde{A}}t},$$

where  $D_{\tilde{A}}$  is the diagonal matrix with diagonal entries equal to those of  $\tilde{A}$  and  $P$  is the polynomial:

$$P(t) = \begin{pmatrix} 1 & \frac{1}{2}t + \frac{a-1}{2\sqrt{1-w^2}} \\ 0 & t \end{pmatrix}. \quad (3.3)$$

This nice factorization is, in fact, a consequence of the Hermitian character of the function  $\chi$ .

Thus, we seem to have succeeded in finding a situation where *the solution of an instance of Dirac's equation is directly related to a weight matrix allowing for a symmetric second order differential operator with matrix coefficients.*

But this is not yet the case.

Although the weight matrix  $W = e^{-t} T T^*$  satisfies the differential equations (2.5) and (2.6) for

$$\begin{aligned} A_2(t) &= tI, \\ A_1(t) &= \begin{pmatrix} -1 - (1 + 2\sqrt{1-w^2})t & -1 + 2a + 2\sqrt{1-w^2}t \\ 0 & 1 + (-1 + 2\sqrt{1-w^2})t \end{pmatrix}, \\ A_0 &= \begin{pmatrix} 1 - 2\sqrt{1-w^2} & -\frac{1}{2} + \sqrt{1-w^2} \\ 0 & 0 \end{pmatrix}, \end{aligned}$$

the second order differential operator

$$\ell_2 = A_2 D^2 + A_1 D + A_0 D^0$$

is not symmetric for  $W$  because  $W$  does not satisfy the boundary conditions (2.3). More precisely, the weight matrix  $W$  is not integrable at  $t = 0$ . That means that one cannot associate a sequence of orthogonal polynomials to  $W$ .

However, a bit of extra work will allow us to make the desired connection.

Indeed, it is straightforward to check that the polynomial  $P$  (see (3.3)) which appears in the factorization of  $T$ , satisfies the first order differential equation

$$P'(t) = \frac{1}{t} \begin{pmatrix} 0 & \frac{1}{2} \\ 0 & 1 \end{pmatrix} P(t).$$

For  $\alpha > -1$ , we associate with the matrix  $E = \begin{pmatrix} 0 & \frac{1}{2} \\ 0 & 1 \end{pmatrix}$  the matrix

$$E_0 = \frac{1 + \alpha}{5} \begin{pmatrix} -1 & 1/2 \\ -2 & 1 \end{pmatrix}.$$

They satisfy that  $EE_0 - E_0E = E_0$  and  $E_0^2 + \alpha E - E_0$  is Hermitian. According then to section 6.2 of [DG1], we have that the weight matrix  $t^\alpha e^{-t} P(t) H P^*(t)$ , where  $H = P^{-1}(1)(P^{-1})^*(1)$ , goes along with the following symmetric second order differential operator

$$\ell_2 = tD^2 + (-tI + 2E + (\alpha + 1)I)D + (-E + E_0)D^0.$$

The space of second order differential operators that have the corresponding orthogonal polynomials as their common eigenfunctions is of dimension *four*. Among these there is a three-dimensional subspace consisting of operators that are *symmetric* with respect to the inner product given by  $W(t)$ , one of which is displayed above. These operators and the weight  $W(t)$  necessarily satisfy the conditions (2.3), (2.4), (2.5), (2.6) above. There is a differential operator of order 2, linearly independent from these ones that is *not symmetric*. There is of course one trivial operator of order zero: the identity. This situation is very similar to the one encountered in several examples in [CG].

The orthogonal polynomials with respect to the weight matrix  $t^\alpha e^{-t} P(t) H P^*(t)$  have been studied in more detail, including a Rodrigues' type formula, a three term recurrence relation, other symmetric second order differential operators for the weight matrix, etc. in [DL].

The weight matrix here, which is independent of  $a$ , and the one in [DL] in the case  $a = 1/2$ , are related by a simple conjugation by the unitary matrix

$$\begin{pmatrix} \frac{1}{\sqrt{5}} & \frac{2}{\sqrt{5}} \\ -\frac{2}{\sqrt{5}} & \frac{1}{\sqrt{5}} \end{pmatrix}.$$

Summarizing, we have the following theorem.

**Theorem 3.1.** Consider the following instance of the de Dirac equation  $T' = (\tilde{A} + \tilde{B}/t)T$ , where

$$\tilde{A} = \sqrt{1 - 1/(4a)^2} \begin{pmatrix} -1 & 1 \\ 0 & 1 \end{pmatrix}, \quad \tilde{B} = \begin{pmatrix} -1/2 & a - 1/2 \\ 0 & 1/2 \end{pmatrix},$$

and its solution

$$T(t) = t^{-1/2} \begin{pmatrix} e^{-\sqrt{1-1/(4a)^2}t} & \left(\frac{1}{2}t + \frac{a-1}{2\sqrt{1-1/(4a)^2}}\right) e^{\sqrt{1-1/(4a)^2}t} \\ 0 & t e^{\sqrt{1-1/(4a)^2}t} \end{pmatrix}.$$

Then for each  $\alpha > -1$ , the weight matrix

$$W = t^{\alpha+1} e^{-t} T(t) e^{-D_{\tilde{A}}t} H e^{-D_{\tilde{A}}^*t} T^*(t),$$

where  $H = e^{D_{\tilde{A}}} T^{-1}(1)(T^{-1})^*(1) e^{D_{\tilde{A}}^*}$ , allows for the following symmetric second order differential operator

$$\ell_2 = tD^2 + (-tI + 2E + (\alpha + 1)I)D + (-E + E_0)D^0,$$

where

$$E = \begin{pmatrix} 0 & \frac{1}{2} \\ 0 & 1 \end{pmatrix}, \quad E_0 = \frac{1 + \alpha}{5} \begin{pmatrix} -1 & 1/2 \\ -2 & 1 \end{pmatrix}.$$



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